Modeling and Simulation of Polysilicon Piezoresistors in CMOS-MEMS Resonator for Biomarker Detection in Exhaled Breath

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***Abstract*—This research studies longitudinal and transverse polysilicon resistors deposited in the maximum stress points of a CMOS-MEMS resonator for mass detection. The longitudinally mounted resistors were found to increase with the stress and giving maximum of resistance change of 10 to 23 Ω when the actuation voltage was varied from 50 to 180 V, while the transverse resistors were found to decrease from 0.8 to 0.4 Ω for the given voltages. Possible Wheatstone bridge configurations were studied to get the maximum output voltage, which was found to be 14 mV when two equal longitudinal resistors are connected with two equal external resistors to form a half bridge configuration.**

Keywords-piezoresistance; biomarkers; exhaled breath

I. INTRODUCTION

Piezoresistors are used in MEMS resonators and pressure sensors as sensing elements to detect any small changes in the stress. Piezoresistivity of materials is described by coefficients called π- coefficients or piezoresistance coefficients. In general case, 81 coefficients are needed, however for silicon only three (π_{11}, π_{12}, π_{44}) are needed due to the symmetry in the silicon crystal. The sensitivity of the piezoresistor to the applied stress or strain depends on the orientation of the resistor relative to the components of the stress and the strain, and it also depends on the crystal type [1]. The change ΔR in a piezoresistor with a nominal value R is proportional to the strain ε and it can be given by (1) below.

$$\Delta R = G\varepsilon R \tag{1}$$

The proportionality constant G is called a gauge factor of the piezoresistor, and it depends on the orientation of the resistor and the direction of the applied stress. The relative change of the measured resistance to the longitudinal strain is called longitudinal gauge factor, while the relative change in the resistor to the transverse strain is called transverse gauge factor [2]. A resistor R with length l_r, width w_r, thickness t_r and resistivity ρ_r can be found using (2).

$$R = \frac{\rho_r l_r}{w_r t_r} \tag{2}$$

By taking differentiation of (2) we get

$$\frac{\Delta R}{R} = \frac{\Delta \rho_r}{\rho_r} + \frac{\Delta l_r}{l_r} - \left[\frac{\Delta w_r}{w_r} + \frac{\Delta t_r}{t_r}\right] \tag{3}$$

Equation (3) shows that the change includes the piezoresistor geometry change in addition to the change in the piezoresistor resistivity.

A. *Uniaxial stress*

A mounted piezoresistor on an axially stressed beam undergoes longitudinal and transverse resistivity changes as a function of the applied strain. Equations (4) and (5) show the resistivity strain relation [3].

$$\left(\frac{\Delta \rho_r}{\rho_r}\right)_L = g_L \varepsilon_L \tag{4}$$

$$\left(\frac{\Delta \rho_r}{\rho_r}\right)_T = g_T \varepsilon_L \tag{5}$$

where g_L and g_T are longitudinal and transverse gauge factors, respectively, ε_L and ε_T are longitudinal and transverse strains, respectively. g_L and g_T are related to the π-coefficients as below.

$$g_L = \pi_l E \tag{6}$$

$$g_T = \pi_T E \tag{7}$$

where E is the Young's modulus, π_l and π_T are longitudinal and transverse piezoresistance coefficients. For the longitudinal stress, (3) can be rewritten as

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$$\left(\frac{\Delta R}{R}\right)_L = \left(\frac{\Delta \rho_r}{\rho_r}\right)_L + \varepsilon_L - \varepsilon_T - \varepsilon_Z \qquad (8)$$

where the longitudinal strain ε_L is the change in the length, the transverse strain ε_T is the change in the width and ε_z is the strain in the thickness of the piezoresistor and it is equal to ε_T . From hook's law, the transverse strain caused by longitudinal load are related to the longitudinal strain by Poisson's ratio υ as shown by (9) [4].

$$\varepsilon_T = \varepsilon_z = -\upsilon\varepsilon_L \qquad (9)$$

By substituting (9) in (8), the change in the resistance of the piezoresistor due to longitudinal stress can be written as below.

$$\left(\frac{\Delta R}{R}\right)_L = \left(g_L + 1 + 2\upsilon\right)\varepsilon_L = G_L\varepsilon_L \qquad (10)$$

where G_L is the total gauge factor found by considering change of the piezoresistor resistivity in addition to its geometry change, and it is found by (11).

$$G_L = g_L + 1 + 2\upsilon \qquad (11)$$

When the mounted piezoresistor is transversely stressed the transverse strain is still same as the strain in the thickness of the piezoresistor, and the total transverse strain of the piezoresistance change can be expressed as below.

$$\left(\frac{\Delta R}{R}\right)_T = \left(\frac{\Delta \rho_r}{\rho_r}\right)_T + \varepsilon_T - \varepsilon_L - \varepsilon_Z = G_T\varepsilon_L \qquad (12)$$

where G_T is the total transverse gauge factor found by considering changes in both resistivity and geometry of the piezoresistor and given by (13).

$$G_T = \left(\frac{\Delta R}{R}\right)_T \Big/ \varepsilon_L = g_T - 1 \qquad (13)$$

It can be seen from above equations that g is the gauge factors associated with the resistivity changes only, while G is the gauge factors which include resistivity in addition to the geometry changes. By substituting g_L and g_T from (6) and (7) into (11) and (13), the total longitudinal and transverse gauge factors are found as in (14) and (15), respectively.

$$G_L = \pi_L E + 1 + 2\upsilon \qquad (14)$$

$$G_T = \pi_T E - 1 \qquad (15)$$

By looking at (14) and (15), the gauge factor in (14) has a component $\pi_L E$ due to the resistivity change and a component $1+2\upsilon$ due to the geometry change, and in (15) the gauge factor has $\pi_T E$ from the resistivity change and -1 from the geometry change. G due to geometry changes is very small compared to the G from the resistivity change in the semiconductor materials such as silicon, hence the geometry change can be neglected [5] and (14) and (15) are written as

$$G_L = \pi_L E \qquad (16)$$

$$G_T = \pi_T E \qquad (17)$$

B. π - Coefficients of polysilicon

Polysilicon is considered as a composition of crystalline grains of silicon separated by grain boundaries, and they behave like the single crystal silicon. Longitudinal and transverse piezoresistance coefficients for randomly oriented polysilicon grains can be estimated by (18) and (19) below [1].

$$\pi_L = \pi_{11} - 0.400(\pi_{11} - \pi_{12} - \pi_{44}) \qquad (18)$$

$$\pi_T = \pi_{12} + 0.133(\pi_{11} - \pi_{12} - \pi_{44}) \qquad (19)$$

The above longitudinal and transverse piezoresistance coefficients for the randomly oriented p-type and n-type polysilicon are given in TABLE I below [1].

TABLE I. PIEZORESISTANCE COEFFICIENTS FOR POLYSILICON

Parameter	p-type polysilicon	n-type polysilicon
π_L	58.8×10^{-11}/Pa	-45.4×10^{-11}/Pa
π_T	-18.5×10^{-11}/Pa	34.5×10^{-11}/Pa

C. Wheatstone bridge for small resistance change measurement

The small changes in the piezoresistance is translated and measured as a voltage using a simple Wheatstone bridge [6]. Wheatstone bridge uses four resistors configured in the four arms of the bridge. Depending on the number of the active resistors (transducer), quarter bridge (one transducer), half bridge (two transducers), and full bridge (four transducers) of the Wheatstone bridge can be used as shown in Fig. 1. The quarter bridge (Fig. 1(a)) uses only one active element R_3 which changes due a physical phenomenon such as pressure, force, temperature...etc., while the rest of the resistors are passive. The change ΔR_3 in R_3 is proportional to the measured physical quantity. However, the output voltage of this configuration is nonlinear as described by (20) [7].

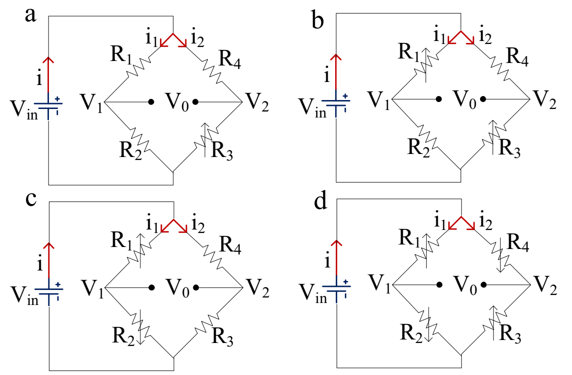

Figure 1. Wheatstone bridge configuration types, (a) quarter bridge, (b and c) half bridge, and (d) full bridge configurations

$$V_0=V_2-V_1=\left(\frac{R_3+\Delta R_3}{R_3+R_4+\Delta R_3}-\frac{R_2}{R_1+R_2}\right)V_{in} \qquad (20)$$

The half bridge uses two active elements. The two active elements should be placed in diagonal of the bridge (Fig. 1(b)) if both elements have the same response to the quantity being measured. The output voltage is double that of the quarter bridge, however it is also nonlinear as shown in (21).

$$V_0=V_2-V_1=\left(\frac{R_3+\Delta R_3}{R_3+R_4+\Delta R_3}-\frac{R_2}{R_1+R_2+\Delta R_1}\right)V_{in} \qquad (21)$$

To have a linear output for the half bridge circuit identical active elements with opposite response to the measured physical quantity are configured in the same branch of the bridge as shown by Fig. 1(c). Equation (22) shows the output voltage of this configuration and it is linear when $R_1 = R_2$.

$$V_0=V_2-V_1=\left(\frac{R_2-\Delta R_2}{R_1+R_2+\Delta R_1-\Delta R_2}-\frac{R_3}{R_3+R_4}\right)V_{in} \qquad (22)$$

The full bridge configuration uses four active elements. The best placement of the resistors in this configuration is to put every two resistors with the opposite response to the measured quantity in one branch of the bridge as shown by Fig. 1(d). Due to stress, R_1 and R_3 increase by ΔR_1 and ΔR_3, while R_2 and R_4 decrease by ΔR_2 and ΔR_4, respectively. The output voltage of full bridge configuration can be written as in (23).

$$V_0=\left(\frac{R_3+\Delta R_3}{R_3+R_4+\Delta R_3-\Delta R_4}-\frac{R_2-\Delta R_2}{R_1+R_2+\Delta R_1-\Delta R_2}\right)V_{in} \qquad (23)$$

This configuration is the best compared to the quarter and the half bridge circuits when the four resistors are equal as in (23), and it is analysed in details in the following sections.

II. Modeling of the Polysilicon Piezoresistors

Fig. 2 shows a sketch of a fabricated resonator for biomarker detection in exhaled breath, using p-type polysilicon resistors as sensing elements besides a capacitive sensing. The design consists of two structures (fixed structure (Fig. 2(a)) and a movable structure (Fig. 2(b)) to put on top of the fixed structure. The fixed structure contains three rectangular plates. Two plates are used for actuation and one plate is used for sensing. The movable structure is a square plate made only of 0.35 CMOS technology layers and it is supported by four long flexible beams. The center square plate contains plates same as the ones in the fixed structure to form actuation and sensing capacitors. A sensitive material to the targeted biomarker is deposited on the back side of the movable square plate. Four p-type polysilicon resistors (R_1, R_2, R_3 and R_4) were deposited on the anchor points of the resonator where the stress is the maximum. R_1 and R_3 are identical resistors and they were embedded longitudinally, while R_2 is equal to R_4 and they were transversely mounted.

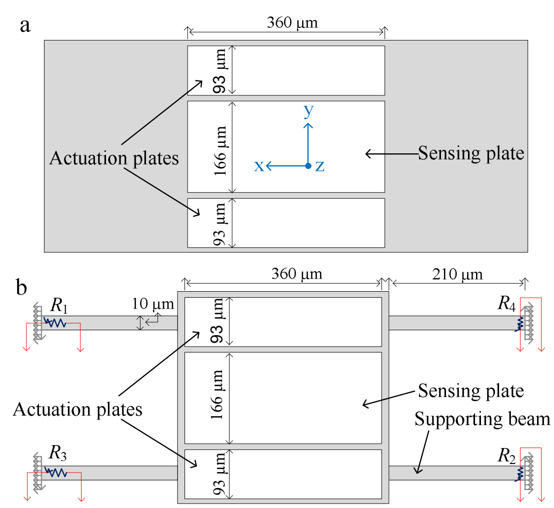

Figure 2. Schematic of the proposed resonator for biomarker detection in exhaled breath showing the (a) the fixed structure and (b) the movable structure with the actuation and sensing plates

By knowing the dimensions of the deposited polysilicon piezoresistors and the resistivity ρ_r or the sheet resistance R_s of the polysilicon, the values of the embedded resistors can be found using (24) and (25).

$$R=\frac{\rho_r l_r}{w_r t_r}=R_s\frac{l_r}{w_r} \qquad (24)$$

$$R_s = \frac{\rho_r}{t_r} \quad (25)$$

The design is fabricated using 0.35 CMOS technology, MIMOS Berhad, Malaysia. This technology uses p-type polysilicon resistors with 87 Ω/□ sheet resistance and 0.285μm thickness. From (25) the resistivity of polysilicon was calculated and found to be $2.48\times10^{-5}\Omega.m$. TABLE II shows the dimensions and the values of the embedded piezoresistors found by using above equations.

TABLE II. DIMENSIONS OF THE EMBEDDED POLYSILICON RESISTORS

Parameter	Value			
	R_1	R_2	R_3	R_4
Length, l_r (μm)	44	10	44	10
Width, w_r (μm)	2	4	2	4
Thickness, t_r (μm)	0.285	0.285	0.285	0.285
Resistance, R(Ω)	1914	217.5	1914	217.5

A. Stress and resistance change

The electrostatic force generated due to the applied actuation voltage causes a stress on the piezoresistors. All the four piezoresistors will experience longitudinal and transverse strains at the same time. However, depending on the orientation of the stress, longitudinal strain or transverse strain may dominate [2]. The relative change in the longitudinal resistors R_1 and R_3 are found from (10) and (16), while the relative change in the transverse resistors R_2 and R_4 is obtained from (12) and (17). Equations (26) and (27) below give the relative changes in the longitudinal and the transverse resistors, respectively.

$$\frac{\Delta R_L}{R_L} = \pi_L \varepsilon_L E \quad (26)$$

$$\frac{\Delta R_T}{R_T} = \pi_T \varepsilon_L E \quad (27)$$

The electrostatic actuation applies a normal stress in the z direction on the square plate. This stress causes a tensile effect in the x axis for all the supported beams. Due to this normal stress the square plate is displaced and the four supported flexible beams will experience an equal tension (axial stress σ_L) and hence the resulted strain ε_L on the beams is found using (28) [3].

$$\varepsilon_L = \frac{3F_e l_b}{4Ew_b t_b^2} \quad (28)$$

where F_e is the applied electrostatic force, l_b , w_b and t_b are the length, width and thickness of each supported beam. Each beam is a composite of a thin film of three aluminium metal layers, three silicon dioxide layers. By substituting (28) into (26) and (27), the relative change in the longitudinal and transverse piezoresistors can be rearranged as given by (29) and (30), respectively.

$$\frac{\Delta R_L}{R_L} = \pi_L \frac{3F_e l_b}{4w_b t_b^2} \quad (29)$$

$$\frac{\Delta R_T}{R_T} = \pi_T \frac{3F_e l_b}{4w_b t_b^2} \quad (30)$$

The required electrostatic force F_e responsible for exerting the plate displacement depends on the voltage difference applied between the actuation plates as given by (31).

$$F_e = \frac{1}{2}\frac{\varepsilon_0 A_a}{(z_0-z)^2} V_a^{\,2} \quad (31)$$

where $\varepsilon_0 = 8.85\times10^{-12}$ F/m is the permittivity of the free space, A_a is the area of the actuation plates, z_0 is the initial gap between the movable and fixed actuation plates, z is the displacement of the plate and V_a is the voltage difference between the plates. By substituting (31) into (29) and (30) the change in each longitudinal resistor and each transfer resistor can be found by (32) and (33), respectively [8].

$$\frac{\Delta R_L}{R_L} = \pi_L \frac{3l_b}{16w_b t_b^2}\frac{\varepsilon_0 A_a}{(z_0-z)^2} V_a^{\,2} \quad (32)$$

$$\frac{\Delta R_T}{R_T} = \pi_T \frac{3l_b}{16w_b t_b^2}\frac{\varepsilon_0 A_a}{(z_0-z)^2} V_a^{\,2} \quad (33)$$

The changes in the longitudinal and transverse piezoresistors for different initial gap distances (5 μm, 6 μm…up to 10 μm) between the capacitor plates at different applied voltages were found using (32) and (33) and given in Figs. 3 and 4, respectively. It is clear that the resistance change of the longitudinal resistors increase with the stress increase due to the positive longitudinal piezoresistance coefficient, while the transverse resistors decrease because the transverse piezoresistance coefficient is negative. The maximum applied actuation voltage for each gap is limited by the pull in voltage; hence the range taken was different for the individual gaps. The output voltage V_0 of the full bridge configuration using V_{in} as 5 V was found from (23) and given in Fig. 5 for the different gaps at different actuation voltages.

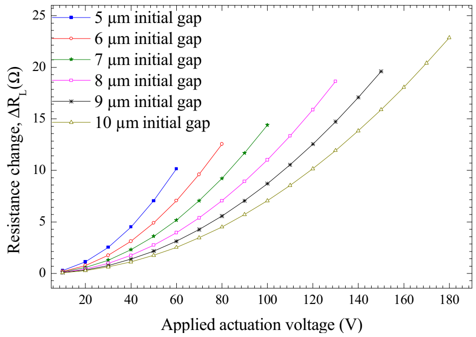

Figure 3. Resistance change for longitudinal resistor at different actuation voltages

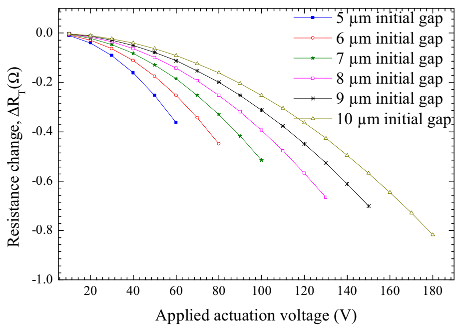

Figure 4. Resistance change for transverse resistor at different actuation voltages

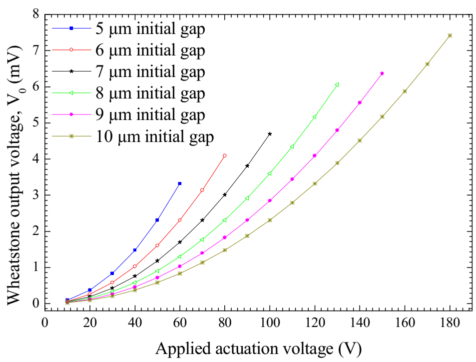

Figure 5. Output voltage of full bridge configuration for the p-type polysilicon resistors at different actuation voltages

Fig. 5 shows that the output of the Wheatstone bridge depends on the applied actuation voltage. Higher applied voltage causes higher stress and as a result higher output response is achieved. For the same actuation voltage different gaps give different responses. Smaller gaps give higher response because the electrostatic force is inversely proportional to the gap as shown in (31).

B. Study of differebridge configurations for maximum output voltage

1) Quarter bridge configuration using three equal external resistors: From (20), when $R_1 = R_2 = R_3 = R_4 = R_L$ and R_3 is the only active resistor, the output voltage is

$$V_0 = V_2 - V_1 = \frac{R_L \Delta R_L}{4R_L^2 + 2\Delta R_L} V_{in} \qquad (34)$$

2) Half bridge configuration using two equal external resistors: By setting $R_1 = R_2 = R_3 = R_4 = R_L$ in (21)and considering , R_1 and R_3 as the only active resistors, the output voltage is

$$V_0 = V_2 - V_1 = \frac{\Delta R_L}{2R_L + \Delta R_L} V_{in} \qquad (35)$$

The output voltage of the all possible configurations at different actuation voltages (10-60 V) for the fixed initial gap between the moving and the fixed structures as 5 µm were found and plotted in Fig. 6. It is clear that the output (Half bridge) of the half bridge configured as in Fig.1 (b) has higher response than the output (Quarter bridge) of the quarter bridge configured by Fig.1 (a) and the output (Full bridge) of the full bridge configured by Fig. 1(d). The full bridge configuration gives the best response when all the four resistors have have same value, however due the difference between the transverse and the longitudinal resistor values as in TABLE III, The full bridge gave the worst response among the three possible configurations for this resonator. As a result the half bridge shown by Fig. 1(b) is recommended to achieve the highest response for this research.

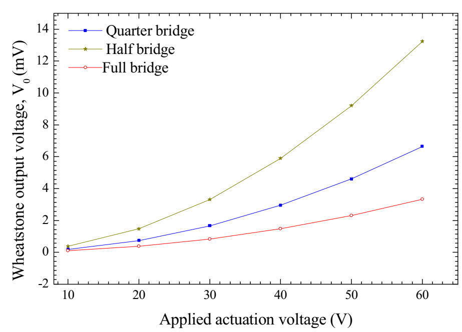

Figure 6. Output voltage for different Wheatstone bridge configurations at different actuation voltages for 5 µm initial gap

III. SIMULATION OF THE LONGITUDINAL PIEZORESISTORS

The modelled resonator shown in Fig. 2 was designed using CoventorWare 2008 software to study the longitudinal piezoresistors for the recommended half bridge configuration at the same actuation voltages (10-60 V) for the same initial gap 5 µm between the moving and the fixed structures. The piezoresistors were simulated and Figs. (7) and (8) show the 3D results of the maximum stress points and the displacement, respectively.

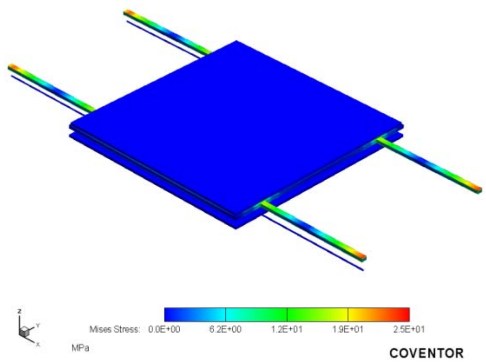

Figure 7. The 3D results showing the maximum atress points colored in red.

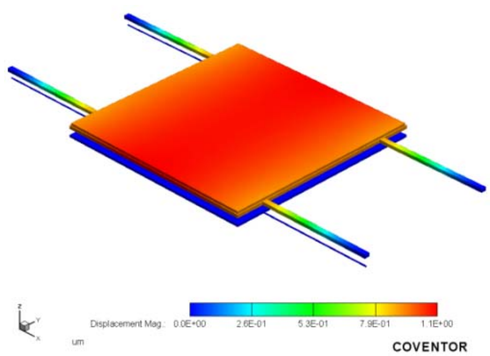

Figure 8. Maximum plate displacement at the center of the plate

TABLE III compares the simulated piezoresistance values with the modelled values for the longitudinal resistors.

TABLE III. SIMULATED AND MODELLED LONGITUDINAL POLYSILICON PIEZORESISTORS

Resistor	Simulated (Ω)	Modelled (Ω)	Error %
R_1	1903.334	1914	0.560
R_3	1903.334	1914	0.560

To study the resistance change in the longitudinal piezoresistor, same actuation voltages given above were used with the same fixed gap, and the resulted resistance changes from the simulation were compared to the modelled resistance changes as shown in Fig. 9. The simulated and modelled longitudinal resistance changes were found to follow the same trend; both increase with the stress increase, and the maximum percentage error difference was found to be around 13% which correspond to the maximum actuation voltage. For the lower actuation voltages the error was very small as in Fig. 9.

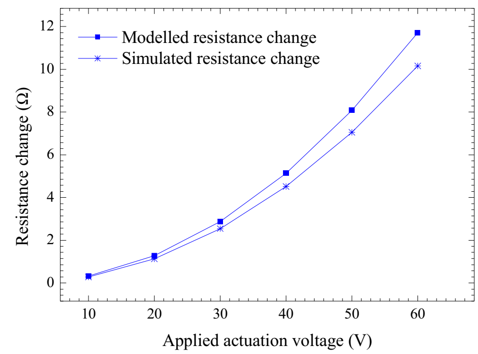

Figure 9. The simulated and modelled resistance change in the longitudinal piezoresistors at different applied voltages for 5 µm initial gap

IV. CONCLUSION

Longitudinal and transverse polysilicon resistors were deposited at the maximum stress points of a CMOS-MEMS resonator to study their resistance change with the stress. It was found that the modelled and simulated longitudinal resistors increase when the stress is increased, while the modelled transverse resistors decrease with the stress. Different Wheatstone bridge configurations were studied and the half bridge configuration was found to give the best output voltage, as big as 14 mV at the maximum possible actuation voltage (60 V) for 5 µm initial gap between the fixed and movable structures. The longitudinal piezoresistors were simulated using CoventorWare 2008 software to find the resistor values and the resistance change due to the applied stress. The simulated results were found to be close to the modelled results within an acceptable error.

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